

March 19, 1965

Dr. W. T. Tutte
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Dear Dr. Tutte:

I have been interested for some time in an application of graph theory to chemical structures. The enclosed materials may help to illustrate the direction of this work.

Part II of the DENDRAL report will be a tabulation of cyclic trivalent graphs through 12 vertices, with some remarks on larger graphs, e.g., the listing of the 16- and 18-vertex polyhedra lacking triangles. As the report may not be so readily accessible to mathematicians I wondered about the utility of publishing this remark as a separate note. Could you suggest what might be an appropriate journal for it?

The Hamiltonian circuits, when present, afford a convenient notation for coding the graphs (as chord lists rotated, etc., to a minimal value). The non-polygonal graphs are much more awkward. I have been looking at them as unions of subgraphs on a least polyhedron. The limiting case is the Hamiltonian circuit, when the underlying "polyhedron" is a circle. I did not know whether this generalization of the Hamiltonian circuit has been thought of before; it might be useful for other computational problems, as it is for the classification of these graphs.

In effect, any subgraph through which a path can be found is labelled (replaced by an edge). The labels can then be mapped as a unique figure of lower order. (I have no proof this is unique, but I so far see no difficulty with a constructive algorithm: reduce any path to a marked edge. In any further reductions if a path traverses a node incident on a marked edge it can be reduced only if it includes the marked edge.)

I do not find this very elegant, and any alternative suggestions you may have for a fundamental classification (and systematic construction) of such graphs would be very helpful.

Indeed, I would appreciate comments or suggestions you may have at any point. I would also be grateful for reprints of any of the many interesting papers you have written in this field. I am constantly running into more of these, and if you have a complete list of your works it would be helpful.

Sincerely yours,

Joshua Lederberg
Professor of Genetics